201-16554U

I U C L I D

Data Set

Existing Chemical	:	ID: 119-06-2
CAS No.	:	119-06-2
EINECS Name	:	di(tridecyl) phthalate
EC No.	:	204-294-3
TSCA Name	:	1,2-Benzenedicarboxylic acid, ditridecyl ester
IUPAC Name	:	di(tridecyl) phthalate
Molecular Formula	:	C34H58O4

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	08.05.2006

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	08.05.2006
Status	:	
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	06.07.2006
Revision date	:	
Date of last update	:	06.07.2006
Number of pages	:	20
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Contact person	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

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1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is not a member of the High Molecular Weight Phthalate Esters subcategory but its data are being used to support a hazard assessment of the subcategory. The subcategory includes eleven CAS numbers (see Freetext).

Remark : This chemical is not a member of the High Molecular Weight Phthalate Esters subcategory but its data are being used to support a hazard assessment of the subcategory. The subcategory includes the following eleven CAS numbers:
68648-93-1 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)
117-84-0 1,2,-benzenedicarboxylic acid, dioctyl ester (DOP)
16883-83-3 1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)
68515-40-2 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)
68515-45-7 1,2,-benzenedicarboxylic acid, dinonyl ester, branched and linear (DNP)
68515-43-5 1,2-Benzenedicarboxylic acid, di-C9-11-branched

and linear alkyl esters (911P)
84-77-5 1,2-benzenedicarboxylic acid, didecyl ester (DDP)
3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (DUP)
85507-79-5 1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)
111381-91-0 1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)
68515-47-9 1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

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1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

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1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

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1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

2.2 BOILING POINT

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

2.5 PARTITION COEFFICIENT

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 2000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: corn oil
Doses	:	
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	
GLP	:	yes
Test substance	:	other TS: ditridecyl phthalate (CAS No. 119-06-2)
Method	:	Test species/strain: Rat/Crj:CD(Sprague-Dawley) Test method: OECD Acute Oral Toxicity Test Route: Oral(Gavage) Doses: 0(vehicle), 2000 mg/kg Number of animals/group: Males, 5; females, 5
Remark	:	Study reports are in Japanese, however, the study summary and data tables are reported in English.
Result	:	No death occurred of either males or females in the treated groups. No effects were found on general condition, body weight changes or autopsy findings. LD50: Male > 2000 mg/kg; Female > 2000 mg/kg
Test substance	:	ditridecyl phthalate (CAS No. 119-06-2). Purity: 93.7-100% (converted by ester value, 198-212).
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

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5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Males, 42 days. Females, from 14 days prior to mating to day 3 of lactation
Frequency of treatm.	:	daily
Post exposure period	:	none
Doses	:	0(vehicle), 10, 50, 250 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL	:	= 10 mg/kg bw
LOAEL	:	= 50 mg/kg bw
Method	:	OECD combined study TG422
Year	:	
GLP	:	yes
Test substance	:	other TS: ditridecyl phthalate (CAS No. 119-06-2)

Method :

Test species/strain: Rat/Crj:CD(Sprague-Dawley)

Test method: OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test

Route: Oral(Gavage)

Doses: 0(vehicle), 10, 50, 250 mg/kg/day

Number of animals/group: 13 Males; 13 Females

Vehicle: Corn oil

Administration period: Males 42 days; Females from 14 days prior to mating to day 3 of lactation

Terminal killing: Males day 43; Females day 4 of lactation

Remark : Study reports are in Japanese, however, the study summary and data tables are reported in English.

Result : No deaths were observed. Increased salivation was transiently observed in male animals of the 50 and 250 mg/kg groups after the day 10 of treatment until the autopsy. No adverse effects were detected on food consumption in males and females of any group, whereas suppression of body weight gain was observed in females of the 50 and 250 mg/kg groups. No adverse effects of ditridecyl phthalate were found on the general condition in females and on body weight gain in males.

Increase in liver weight was observed in males of the 250 mg/kg group and in females of the 50 and 250 mg/kg groups. On histopathological examination of liver, hypertrophy of the centrilobular hepatocytes was observed in males and females of the 50 and 250 mg/kg groups, and catalase positive granules in centrilobular hepatocytes were increased in males, as well. An increase in kidney weight was found in males of the 250 mg/kg group. On histopathological examination, eosinophilic bodies in renal tubular cells were increased in males of the 250 mg/kg group. In addition, basophilic tubules in the cortex which appeared to be regeneration foci resulting from necrosis of renal tubular epithelium were observed in this group. Hyperplasia of the pelvic epithelium and transitional cells of the urinary bladder was found in females of the 250 mg/kg group, while ditridecyl phthalate did not affect kidney weight in females. On urinary testing and hematological examination, no adverse effects of ditridecyl phthalate were noted. On blood chemical examination in males, ALP

activity was found to be increased after the treatment of ditridecyl phthalate at 250 mg/kg.

No testicular toxicity was detected in any groups.

The no observed effect dose level (NOEL) for repeat dose toxicity is considered to be 10 mg/kg/day in males and females.

Test substance : ditridecyl phthalate (CAS No. 119-06-2).
Purity: 93.7-100% (converted by ester value, 198-212)

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
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5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : S. typhimurium TA100, TA1535, TA98, TA1537,
Test concentration : 156, 313, 625, 1250, 2500 and 5000 ug/plate.
Cycotoxic concentr. : >5000 ug/plate
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year :
GLP : yes
Test substance : other TS: ditridecyl phthalate (CAS No. 119-06-2)

Method : Test species/strains: S. typhimurium TA100, TA1535, TA98, TA1537

Test method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Guidelines No. 471

Procedures: Pre-incubation method

Solvent: DMSO

Positive controls: -S9mix: 2-(2-Furyl)-3-(5-nitro-2-furyl)acrylamide (TA100, TA98), Sodium azide (TA1535), 9-Aminoacridine hydrochloride (TA1537)
+S9 mix: 2-Aminoanthracene (all strains)

S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone

Plates/test: 3

Number of replicates: 2

Remark : Study reports are in Japanese, however, the study summary and data tables are reported in English.

Result : This chemical did not induce gene mutations in the S. typhimurium strains. No toxicity was observed up to a concentration of 5000 ug/plate, with or without metabolic activation.

Genetic effects:
S. typhimurium TA100, TA1535, TA98 and TA1537

	+	?	-
Without metabolic activation:	[ ]	[ ]	[*]
With metabolic activation:	[ ]	[ ]	[*]

Test substance : ditridecyl phthalate (CAS No. 119-06-2).
Purity: 99.82%

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
06.07.2006 (1)

Type	:	Escherichia coli reverse mutation assay
System of testing	:	E. coli WP2 uvrA
Test concentration	:	156, 313, 625, 1250, 2500 and 5000 ug/plate
Cycotoxic concentr.	:	>5000 ug/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 472
Year	:	
GLP	:	yes
Test substance	:	other TS: ditridecyl phthalate (CAS No. 119-06-2)
Method	:	Test species/strains: E. coli WP2 uvrA Test method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Guidelines No. 472 Procedures: Pre-incubation method Solvent: DMSO Positive controls: -S9 mix: 2-(2-Furyl)-3-(5-nitro-2-furyl)acrylamide (WP2 uvrA) +S9 mix: 2-Aminoanthracene (all strains) S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone Plates/test: 3 Number of replicates: 2
Remark	:	Study reports are in Japanese, however, the study summary and data tables are reported in English.
Result	:	This chemical did not induce gene mutations in E. coli strains. No toxicity was observed up to a concentration of 5000 ug/plate, with or without metabolic activation.
Test substance	:	ditridecyl phthalate (CAS NO. 119-06-2). Purity: 99.82%
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.07.2006 (1)

Type	:	Chromosomal aberration test
System of testing	:	Chinese hamster lung (CHL) cells
Test concentration	:	0, 1188, 2375, 4750 ug/mL
Cycotoxic concentr.	:	>4750 ug/ml
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473
Year	:	
GLP	:	yes
Test substance	:	other TS: ditridecyl phthalate (CAS No. 119-06-2)
Method	:	Type of cell used: Chinese hamster lung (CHL) cells Test method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Guideline No. 473 Solvent: DMSO Positive controls: -S9 mix: Mitomycin C +S9 mix: Cyclophosphamide

Doses:
-S9 mix(continuous exposure): 0, 1188, 2375, 4750 ug/mL
-S9 mix(short-term exposure): 0, 1188, 2375, 4750 ug/mL
+S9 mix(short-term exposure): 0, 1188, 2375, 4750 ug/mL

S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone

Plates/test: 2

Remark : Study reports are in Japanese, however, the study summary and data tables are reported in English.
Result : Ditridecyl phthalate did not induce structural chromosomal aberrations and polyploidy in CHL cells, with or without an exogenous metabolic activation system.
Test substance : ditridecyl phthalate (CAS No. 119-06-2)
purity: 99.82%
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
06.07.2006 (1)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type	:	One generation study
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Males 42 days; Females from 14 days prior to mating to day 3 of lactation.
Frequency of treatm.	:	daily
Premating exposure period		
Male	:	14 days
Female	:	14 days
Duration of test	:	Males 43 days; Females from 14 days prior to mating to day 4 of lactation
No. of generation studies	:	
Doses	:	0(vehicle), 10, 50, 250 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL F1 offspring	:	= 250 mg/kg bw
other: NOAEL parental (male)	:	= 250 mg/kg bw
other: NOEL parental (female)	:	= 50 mg/kg bw
Method	:	OECD combined repeated dose and reproductive/developmental toxicity screening test
Year	:	
GLP	:	yes
Test substance	:	other TS: ditridecyl phthalate (CAS No. 119-06-2)
Method	:	Test species/strain: Rat/Crj:CD(Sprague-Dawley)

Test method: OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test

Route: Oral(Gavage)

Doses: 0(vehicle), 10, 50, 250 mg/kg/day

Number of animals/group: 13 Males; 13 Females

Vehicle: Corn oil

Administration period: Males 42 days; Females from 14 days prior to mating to day 3 of lactation

Terminal killing: Males day 43; Females day 4 of lactation

Remark : Study reports are in Japanese, however, the study summary and data tables are reported in English.

Result : No adverse effects were observed on copulation, fertility, maintenance of pregnancy, and delivery in any groups.

A statistically significant decrease in live birth index on PND 0, possibly due to poor lactation, was observed in the 250 mg/kg group (87.7 in high dose vs 99.6 in controls).

Viability of neonates on PND 4 was slightly decreased (not statistically significant) in the 250 mg/kg group (89.9 in the high dose vs. 96.8 in controls). However, there were no adverse effects of ditridecyl phthalate on sex ratio, body weight changes, and morphological appearance of pups.

NOAELs for reproductive and developmental toxicity are considered as follows:
250 mg/kg/day in males based on no testicular toxicity observed at any dose, no effect on copulation, and no effect on fertility.
50 mg/kg/day in females based on the observed decreased in live birth index on PND 0 only in the 250mg/kg group.
250 mg/kg/day in pups due to no adverse effects on sex ratio, body weight changes, and morphological appearance of pups.

Test substance : ditridecyl phthalate (CAS No. 119-06-2).
Purity: 93.7-100% (converted by ester value, 198-212)

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

06.07.2006 (1)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Males 42 days; Females from 14 days prior to mating to day 3 of lactation
Frequency of treatm.	:	daily
Duration of test	:	Males 43 days; Females from 14 days prior to mating to day 4 of lactation
Doses	:	0(vehicle), 10, 50, 250 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL teratogen.	:	= 250 mg/kg bw
other:NOEL maternal tox	:	= 10 - mg/kg bw
Method	:	other: OECD combined study TG422
Year	:	
GLP	:	yes
Test substance	:	other TS: ditridecyl phthalate (CAS No. 119-06-2)

Method : Test species/strain: Rat/Crj:CD(Sprague-Dawley)

Remark : Study reports are in Japanese, however, the study summary and data

tables are reported in English.

Result : There were no adverse effects of ditridecyl phthalate on sex ratio, body weight changes, and morphological appearance of pups. The NOAEL for developmental effects in pups was 250 mg/kg/day.

Maternal effects included mild suppression of body weight gain (<10% decrease) and increased liver:body weight ratios in females of the 50 and 250 mg/kg groups. Other than slight liver hypertrophy, there were no adverse histopathologic findings in tissues of female rats. In addition, no adverse effects were observed on copulation, fertility, maintenance of pregnancy, and delivery in any groups. The NOEL for maternal effects was 10 mg/kg/day.

Test substance : ditridecyl phthalate (CAS No. 119-06-2)
Purity: 93.7-100% (converted by ester value, 198-212)

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

06.07.2006 (1)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Japan Ministry of Health & Welfare (unpublished). Toxicity Testing Reports of Environmental Chemicals, Ditridecyl phthalate (CAS No. 119-06-2). hppt://wwwdb.mhlw.go.jp/ginc/cgi-bin/db1_search.pl?CAS=119-06-2.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT